

A Revolution in Engineering

Space-age computers are improving down-to-earth products, making nuclear storage safer, and expanding research frontiers worldwide



Together science and high power computers will make aircraft, automobiles, and a host of products and technologies safer and less expensive

A computer program makes economic predictions and learns from its mistakes

IN THIS ISSUE

1 THE NEW FACE OF ENGINEERING

Computers that make one-trillion calculations per second are changing how engineers work and are moving the trials and errors out of product development and into computer simulation.

2 Citation Impact: Modeling & Simulation Are Taking on the World

Here's how we recognize a winning technology.

4 Simulating Nature to Answer Engineering Riddles

The natural world holds answers to many technological questions.

5 Predicting with Confidence

Researchers face challenges of creating a sort of "crystal ball" that links cutting edge science with high performance computers.

6 Bouncing on Mars

Sandia teams up with NASA to soften the blow of landing equipment on the Red Planet.

From the Abacus to Deep Blue

Computing has been around longer than you may think.

8 A Walk Through the Simulation Process

A step-by-step look at how two simulations arrive at insight

10 MARKETS FOR THE NEXT MILLENNIUM

Manufacturers are capitalizing on advances that national security projects pioneered.

Automated Mesh Generation

A manufacturing technology replicates complex three-dimensional shapes.

12 A SPECTRUM OF USES

The engineering revolution has arrived on Main Street. Americans can expect a host of benefits from better law enforcement to environmental forecasts, from safer transportation to user-friendly medicine.

Economics: Little People, Big Effects

Aspen, a program to model the economy, considers the household as a major economic force.

16 PERSPECTIVE: But is it alive?

Are powerful computers more than just tools?

This issue of *Emergent* addresses a revolution in engineering. Sandia now has the most powerful computer in the world. Called the teraflop, it allows engineers to apply science in such unprecedented detail that the field of engineering is about to undergo a radical shift. From time immemorial, engineers have relied on trial and error to apply knowledge and develop a product or technology. Trial and error requires real-world testing, which is not always an option for designers anymore. For example, the nuclear stockpile must be failsafe, but testing is banned.

High performance computers, such as the teraflop, allow engineers to design, test, analyze, and make predictions about processes, materials, and products with relatively little real-world testing. The New Face of Engineering (pages 1–7) gives background on how engineering and computers have evolved. This section also explains modeling and simulation. Markets for the Next Millennium (pages 10–11) discusses the application of modeling and simulation in the business community, and A Spectrum of Uses (pages 12–16) shows how this revolution touches the lives of most Americans. Throughout, Sandia innovations are highlighted.

Sandia's exploratory research fund (LDRD) has sponsored the science underlying many of the following technologies and projects: • Pathfinder airbags for landing on Mars; • crash-and-burn studies to understand auto and airline disasters; • virtual hostage rescue; • Aspen, a tool for economic forecasting; • the paleo-simulation of a 75-million-year-old dinosaur's voice; • comet-impact simulation; • data mapping, a new way of looking at facts; • predicting the effects of global warming; and • medical simulations.

Laboratory Directed Research and Development (LDRD)

LDRD, Sandia National Laboratories' exploratory research fund, supports national security and enhances Sandia's technology base. This program is dedicated to early exploration and exploitation of innovative concepts that arise during laboratory work.

Emergent is the quarterly publication of the exploratory research office (LDRD) at Sandia National Laboratories, Albuquerque, NM. Emergent team — PROGRAM MANAGER: Chuck Meyers, Sandia National Laboratories; RESEARCHERS: Joy Bemesderfer & Donna Drayer, BE Inc.; WRITER, PAGE LAYOUT: Katharine Beebe, BE Inc. Please direct comments to Chuck Meyers at (505)844-3459 or e-mail: cemeyer@sandia.gov

SAND98-1075

ON THE COVER: The cover illustration shows the three-stage progression of using a supercomputer to create a technology. The concept begins with a real-world example (the human arm). The example is then translated into a computer model, which is tested for feasibility in a process called simulation. The final stage is to build the technology (the robotic arm in the background).

The new *of* face ENGINEERING

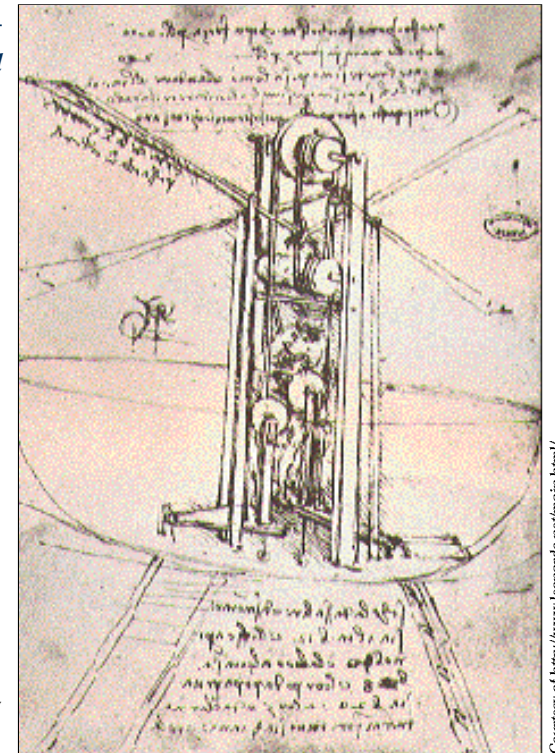
*Tried & true trial & error makes room for
design & testing on the computer screen.*

Stone tools, cathedrals, the cordless phone — the same process created them all: trial and error. We and our ancestors have relied on this process for 2-million years; every era of engineers has followed the same procedure: make it, break it, and make it again better. But that is changing as cutting edge science and high performance computing join forces to revolutionize engineering. The ancient process of invention will never be the same.

Since Leonardo da Vinci conceptualized a flapping wing machine, test pilots have paid with life and limb to advance aviation. Trial and error or trial and terror? By any name it was the dark side of progress. But if people wanted to fly, someone had to test the plane. Similarly, if the sick wanted a second chance at life, someone had to brave the scalpel or swallow a new drug. Until researchers found a substitute for real-world testing, trial and error engineering provided the only way to develop new technologies, products, and procedures.

(Please turn to page 2)

*Increasingly, when failure is not an option or
when benefits far outweigh costs, high
performance computers will help researchers,
engineers, and other professionals make
decisions they can stake lives on.*



Courtesy of <http://www.leonardo.net/main.html/>

LEONARDO'S FLAPPING WING MACHINE
Engineer, architect, inventor, and visual artist Leonardo da Vinci designed numerous flying machines. Especially innovative was the flying saucer, shown here. The pilot's head provided leverage while his hands directed oarlike wings in a cross motion that simulated the gait of a horse.

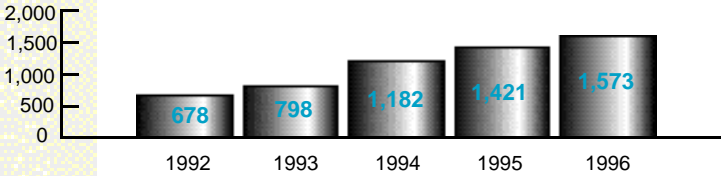
Citation impact: Modeling & simulation are taking on the world

If computer modeling and simulation are revolutionizing engineering, then scientific literature should reflect global interest. Sandia's exploratory research office (LDRD) asked the Institute for Scientific Information (ISI) in Philadelphia to perform an analysis. ISI has a database of 16-million scientific and engineering papers from refereed journals published since 1981. ISI conducted a key-word search for papers published on computer modeling and simulation between 1992 and 1996. The search produced 5,600 papers. The number of papers in 1992 (678) more than doubled by 1996 (1,573). (See bar graph, lower right.)

The United States led in numbers of papers published, with Japan second and England third. When organizations were analyzed for modeling-and-simulation publications, universities and government agencies were found to publish the most. The primary fields where modeling and simulation were applied were in materials science, biochemistry, biomedicine, agriculture, and physics. ISI calculated impact based on how many citations a paper received. The papers with greatest impact discussed applications in biomedicine, biology, and physics.

For more on citation impact, contact David Pendlebury at the Institute for Scientific Information (215) 386-0100; email: dpendle@isinet.com

| Country | # of papers since '92 on Modeling & Simulation |
|---------------|--|
| United States | 1,985 |
| Japan | 694 |
| England | 473 |
| Germany | 390 |
| Canada | 366 |
| France | 280 |
| Netherlands | 237 |
| Australia | 169 |
| Italy | 143 |



The number of papers on computer modeling and simulation from the United States, Europe, Japan, and Australia more than doubled between 1992 and 1996.

(Continued from page 1)

Technology alters the demands of life, work, and leisure overnight. The novelties of yesterday are necessities today. But technology must improve life, not risk it, even though much rests on failsafe performance. Aircraft, for example, flying at once-unimaginable altitudes must be in every way dependable. And automobiles of the future, traveling bumper to bumper at 200 mph, will leave no room for error. The world is embracing ever more inventions that must instill total confidence. And therein lies a challenge: How can we develop inventions that for reasons of safety, cost, environment, etc., cannot be completely tested?

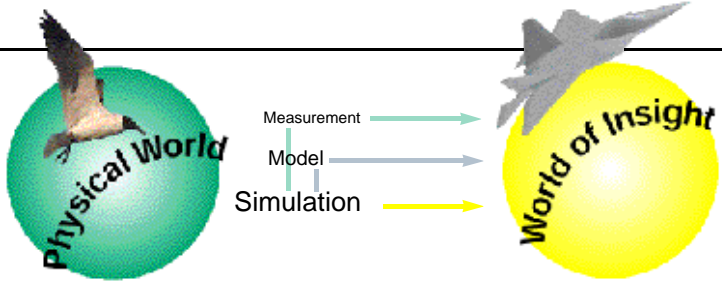
How can we ensure they perform safely and predictably?

Make it and break it 10,000 times — this is modeling and simulation

Greatly refined by high performance computers, two technologies called modeling and simulation are offering a long-needed substitute for real-world testing. *Modeling* means using a computer to depict something from the real world — whether it be an object such as a building, a technology such as a car, a natural phenomenon such as gravity, or a physiological entity such as a brain. The model is described mathematically (numerically) and fed to the computer. The

computer then uses the numerical description like a palette of colors and creates an image — for example, a car. Thus, engineers can look at data converted to three-dimensional form. Next the model is tested for behavior under stress. The stress situation is reenacted — or *simulated*. An aircraft model can fall out of the sky repeatedly till engineers find the problem. Similarly, a surgeon can “operate” on a model brain — make 1,000 deadly slips till a technique is perfect.

As before, engineers still design, build, test, refine. They still make it, break it, and make it better, but they do most of this on the computer screen. Using today’s powerful computers, engineers are test-wrecking more flying machines than Leonardo ever dreamed of, but these crashes take no lives. The space program kicked off this revolution, and the nuclear test ban, which prohibits nuclear explosions in the air, outer space, and under ground, is leading to further breakthroughs. Both cases prohibited actual testing because of safety hazards and cost. Yet space exploration and nuclear stockpile stewardship urgently require a means to learn the results of errors and accidents. The DOE Accelerated Strategic Computing Initiative, in developing the teraflop computer, provides us the capability to begin modeling the aging nuclear



stockpile, so we can assure the safety, security, and reliability of the stockpile without real-world tests.

Life-cycle engineering

Life-cycle engineering of a product is analogous to the life cycle of a living thing — birth, life, and death. In a similar way, a product is “born” when it is designed and manufactured, it “lives” during its operation and maintenance, and it “dies” when it is no longer functional and must be dismantled and disposed of. Traditional product engineering focuses on birth and also on life, with less concern on product death. For the nuclear stockpile (and increasingly other commercial products), the entire life cycle is of concern.

The revolution in engineering applies to the entire product life cycle. It is a predictive approach to making product development decisions based primarily on science-based, high fidelity, accredited models. Decisions at each stage of the life cycle are made using an interactive working environment in which information, computing, and simulation technologies flow seamlessly across each stage. This

interactive working environment is accessible from any authorized location, and information is captured in a format for future reference and reuse.

The benefits include potential for faster, better, and cheaper products by • decreasing time for a product to reach the market, • allowing design trade-offs early in development, • creating designs that are optimized, • developing innovative concepts, • and offering products that will perform and age predictably.

Increasingly, when failure is not an option (as in nuclear stockpile maintenance, and aircraft and space travel) or when benefits far outweigh costs (as in medicine), high performance computers will help researchers, engineers, and other professionals make decisions they can stake lives on.

(Please turn to page 4)

FLAPPING WINGS: A LESSON IN TRIAL AND ERROR

Historical highlights on muscle-driven flying machines demonstrate the failure and peril of trial-and-error engineering. Note that as designers began to address the wing-surface-to-body-weight ratio, they designed machines that required greater-than-human strength to control. In China, rocket-powered flight starts in the 16th century when a man launches himself and a kite — into oblivion.

c. 1500

Leonardo da Vinci designs flapping wing machines. He never takes a test flight.

c. 1660

A French tightrope walker attempts to demonstrate a winged device for the court of Louis XIV. The small surface area of wing requires rapid flapping. The pilot tires, falls, and is seriously injured.

1678

A French locksmith has modest success with a pair of muslin wings attached to arms and legs. Ultimately, if he jumps from a place above, he is able to glide in a retarded fall over a house roof, but he never achieves sustained flight.

1742

The Marquis de Bacqueville attempts to “fly” over the Seine River in France — about 500 to 600 feet — by flapping wings on his arms and legs. The wing surface area is too small to support his weight; soon after take-off, he becomes exhausted, falls into a barge, and breaks a leg.

1812

J. Degen, a Viennese clockmaker, creates a device with two large umbrella-like wings attached to a central frame, all of which dangles from a hot air balloon. During demonstrations in Paris, the wind blows him out of control. After the third attempt, frustrated spectators beat him up.

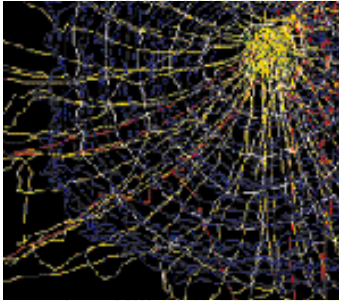
1854

An aeronaut, named Letur, is seated below a giant umbrella-like glider. Separate side wings and tail are supposed to add maneuverability. The glider hangs tethered 80 feet below a balloon. On its descent, the wind slams the glider into trees. The aeronaut dies of his wounds.

1874

A Belgian shoemaker tests an umbrella structure having two 24-foot wings and a 20-foot tail. The apparatus is tethered to a balloon. At 1,000 feet above ground, the pilot disconnects the tether. The wings collapse, the machine crashes, and the shoemaker dies on impact.

SIMULATING NATURE TO ANSWER ENGINEERING RIDDLES



From the website of Dr. Samuel Zschokke, University of Basel, Switzerland

Nature has clever ways of solving problems that befuddle engineers. Consider the spider web — a sort of sticky, loose-weave textile that gums up airborne insects. Engineers have yet to design a comparable structure, such as a fishing net that can snag an airplane.

Before computerized simulation became available, no one could explain the strength of a spider web.

Recently, however, researchers adapted a computer program for crash-testing automobiles to create a spider web model. Defining data included web fiber strength, how the fibers were connected, and how fast insects were flying when they hit the web. Scientists were able to distort the modeled web and analyze the distortions.

What engineers found they would not have guessed: Web fibers less than one-thousandth of a millimeter in diameter created air resistance. Wind and subsequent bobbing from the insect collision had a dampening effect and distributed the force of impact. The web flexed instead of breaking.

For the first time in 400-million years, the spider's secret is out. □

If two heads are better than one, imagine what thousands can do

When they face overwhelmingly complex problems, individuals often form groups to resolve their dilemmas. Organized as a community, ordinary people accomplish the extraordinary. That works for computers too.

In January 1997, Sandia acquired the most powerful computer in the world. It's called the teraflop, and it performs one-trillion calculations per second. It was developed in partnership with Intel Corp. for the Department of Energy to safeguard the world's stockpile of nuclear weapons.

But the teraflop is not exactly a computer; it's thousands — a community of sorts. Nearly 10,000 Intel Pentium Pro™ processors (the same equipment standard desktop computers use) collaborate to create simulations of unprecedented accuracy and to apply scientific principles at unprecedented levels of detail. Extremely complex events can be simulated. A hypothetical nuclear reactor, for example, can melt down in the virtual world of the teraflop. Researchers can use re-enactments — or simulations — to predict cause and outcome and, thus, prevent disaster.

The teraflop does in one second what a person with a calculator would need 30,000 years to do.

Although the computer is styled after a brain, it isn't one. It doesn't think *per se*; it doesn't

react to facts with happiness or outrage. But it can navigate through oceans of data that would drown human intellect. Like Hal in the movie *2001*, the teraflop has an awesome — if artificial — intelligence. But unlike Hal, the teraflop solves, rather than creates, problems.

Modeling and simulation are an evolution as much as they are a revolution, said Sandian David Crawford. "We've been moving in that direction for a long time — since the 1940s," he said. But now equipment allows simulations to leave the one-dimensional world of abstract equations and become three-dimensional images of equations. □

Suggested Reading on modeling and simulation:

Gilen, Kenneth T., & Malone, G. M., "Nuclear power plant accident simulations of gasket materials under simultaneous radiation plus thermal plus mechanical stress conditions." Sandia National Laboratories, July 1997. SAND97-1666.

Sisti, Alex F. "Enabling technology for simulation science." *Proceedings of SPIE — the International Society for Optical Engineering*. 22 – 24 April 1997, Orlando, Florida. V.3083. SPIE, Bellingham, WA. 1997.

Predicting with confidence

One of these days, the crystal ball may be more than a figure of speech. Consider, for example, a Dow-Jones forecast you can bet your bottom dollar on — that would be nice, but first we have some work to do

Life or death decisions: we make them for ourselves, and people — airline pilots, surgeons, money managers — make them for us, spur of the moment choices that *have* to be right. Increasingly, "ball park" estimates won't do. Granted, technology is whittling away at human error, but before we can predict with an accuracy approaching 100%, challenges must be met. The following areas warrant further study:

Computer development

Computing power — one trillion calculations per second for the teraflop — still only allows simplified simulations of complex phenomena. It is too slow for natural systems. For example, to simulate a beating heart, the teraflop slogs through hours of equations to re-enact a single beat.

Simulating nature

The natural world is infinitely complex, and it's constantly changing. Scientists understand basic phenomena — chemical, mechanical, thermal, etc. But engineers need a way to apply that understanding in detail sufficient to recreate natural events and make predictions with accuracy. For example, will a 10,000-acre wildfire destroy a town 40 miles east? Given the cost of evacuation, taxpayers could save hundreds of thousands of dollars if the answer were no.

Also we must learn how nature solves problems, then learn to apply that methodology to technological problems. The economic modeling software Aspen (*see page 12*), for instance, uses the principle of natural selection. Successful economic strategies replicate; those that are not successful die out of the program.

Information packaging

How data are presented determines how useful they are. The world has no dearth of information; indeed, sometimes computers provide so much, it becomes inaccessible unless we find novel ways to package it so researchers can see through the clutter into knowledge and insight (*see Automated Mesh Generation, page 10; and Experiencing Data, page 16*). Also with researchers collaborating worldwide, we must make information accessible to qualified users anywhere, any time. The Internet offers a crude example of a desirable system; however, security, speed, and other factors must be addressed. Users must have confidence they are communicating with whom they believe they are, that files are safe from tampering, and that only authorized users can access the information.

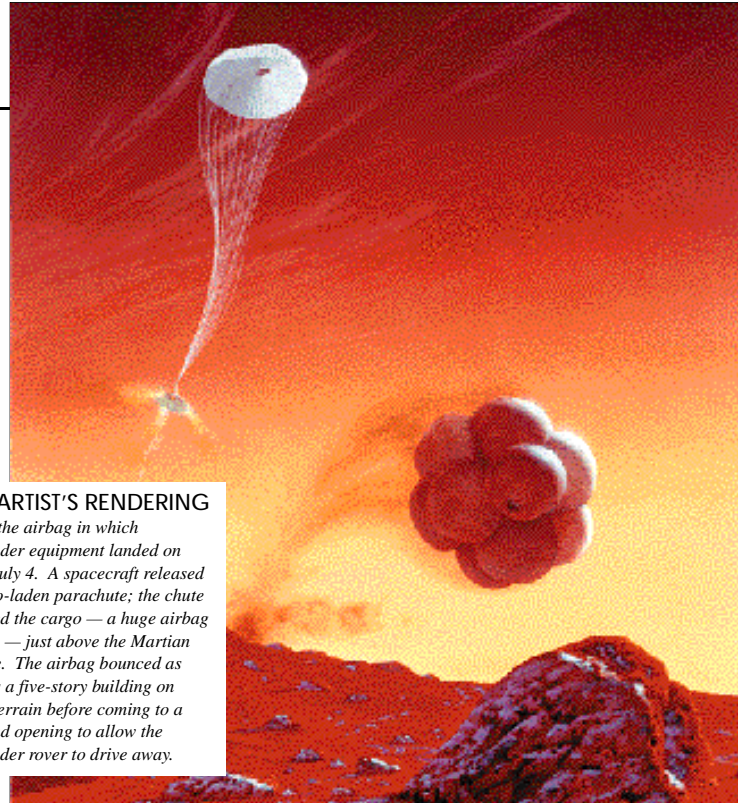
Trusting the simulation

Engineers and researchers must be able to trust simulations. Consider Isaac Newton's real-world test; he dropped an

apple and *saw* it fall. But when we cannot test — for example, with nuclear accidents — and when we cannot witness an event with our eyes and other senses, how can we be sure the simulation reveals truth? What if Newton had simulated, rather than tested, and the apple had risen rather than fallen? If he'd had no real-world experience to compare the simulation to, could he have believed it? Researchers must develop methods to validate simulated results beyond all doubt.

Experimental discovery

Advanced experimental methods must be developed for researchers to make accurate predictions that would, in turn, solve problems. There are key phenomena that cannot be modeled with sufficient accuracy today due to a lack of highly detailed knowledge or experimental data. Experimental discovery of this knowledge is essential. □



THIS ARTIST'S RENDERING shows the airbag in which Pathfinder equipment landed on Mars July 4. A spacecraft released a cargo-laden parachute; the chute released the cargo — a huge airbag cocoon — just above the Martian surface. The airbag bounced as high as a five-story building on rocky terrain before coming to a stop and opening to allow the Pathfinder rover to drive away.

Courtesy of Jet Propulsion Laboratory, NASA Copyright © California Institute of Technology, Pasadena, CA. All rights reserved. Based on government-sponsored research under NAS7-1260.

Bouncing on Mars

Sandia helps NASA and industry design a soft landing for Pathfinder, the Martian probe

Long before author Edgar Rice Burroughs popularized the Red Planet, people have wondered about our neighbor Mars. Now a collaboration between Sandia, NASA, and private industry is helping us fill in some blanks.

On July 4, a small NASARover vehicle landed on Mars to observe rock content, take photographs, and record the weather. NASA's Jet Propulsion Laboratory (JPL) asked Sandia — specifically the parachute laboratory combined with our experience in cargo airdrops and automotive airbags — to design a prototype. Sandia did studies to determine if an airbag containing the rover equipment would survive landing on rocky terrain. Sandia simulated the internal environment of the airbags as they hit the Martian surface and bounced on rocks. To predict if the sensitive instruments would survive the drop to the Martian surface, Sandia created two models. One model studied airbag strength to find out if the bags would be damaged by falling onto rocks. The second model examined air pressure inside the bags when, loaded with cargo, they were dropped onto the rocky surface.

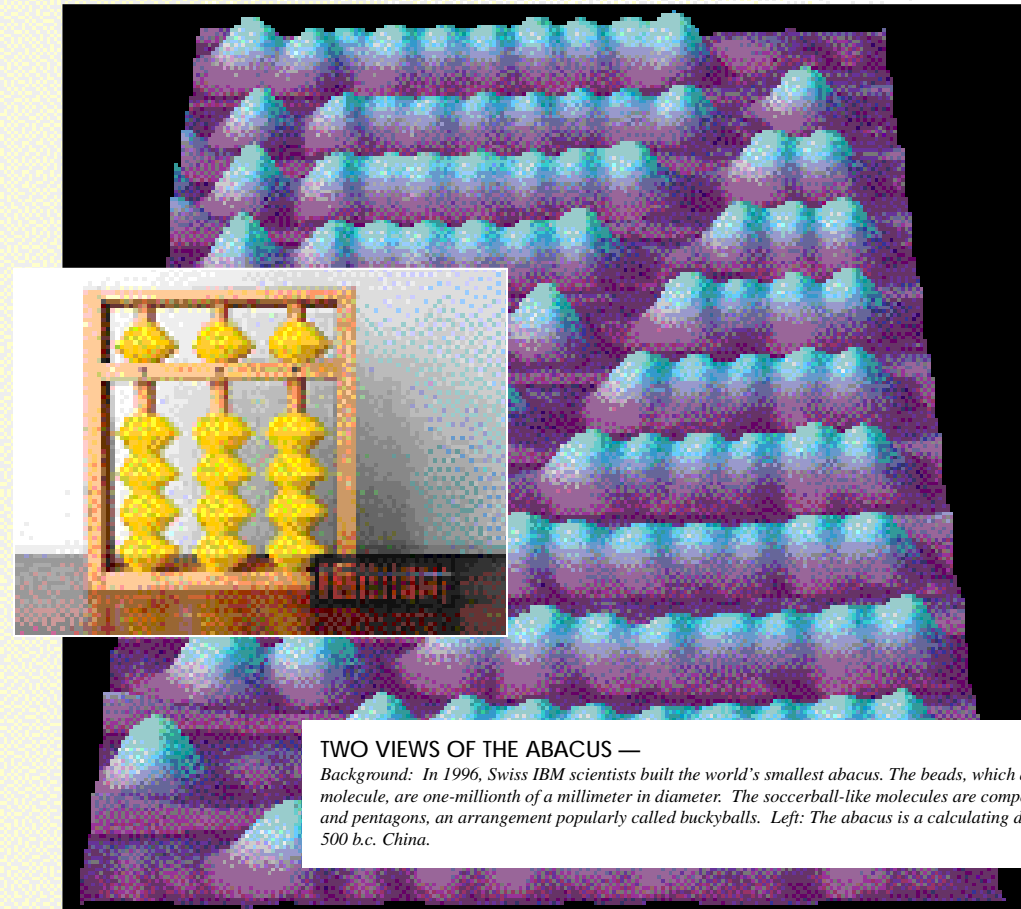
The technology was then turned over to JPL, who contracted with industry to build the airbag and do further testing. As the Sandia models predicted, Pathfinder equipment survived the landing well. □

Suggested Reading: Cole, J. Kenneth, & Wayne, Donald E. *BAG: A code for predicting the performance of a gas bag impact attenuation system for the Pathfinder lander*. Sandia National Laboratories. November 1993. SAND93-2133.

Wayne, Donald E., et al. *MESUR Pathfinder airbag impact attenuation system*. Sandia National Laboratories. August 1994. SAND94-2287A.

ABACUS TO DEEP BLUE

Computing evolves from 17th-century origins



TWO VIEWS OF THE ABACUS —
Background: In 1996, Swiss IBM scientists built the world's smallest abacus. The beads, which are each one molecule, are one-millionth of a millimeter in diameter. The soccerball-like molecules are composed of hexagons and pentagons, an arrangement popularly called buckyballs. Left: The abacus is a calculating device that dates to 500 b.c. China.

FROM THE

The first computer was an abacus, a counting board that performed calculations by sliding beads across rods or grooves. Later, inventions in Renaissance Europe triggered the evolution of computers with a capital C.

1623: German scientists build a calculator that uses sprocketed wheels to add, multiply, and divide; it relies on logarithmic tables.

1642: In France, Blaise Pascal builds an adding and subtracting machine. A 17th-century German mathematician improves Pascal's invention by adding multiplication, division, and determining square roots to its capabilities.

1960s & 1970s: The computer age blossoms with active memory (called RAM), the integrated circuit, and miniaturization.

1963: Digital Equipment introduces the minicomputer.

1970s: Corporations worldwide are using IBM mainframes (computers that accommodate 100 to 500 operators simultaneously).

1975: The personal computer has evolved. IBM produces personal computers that are compatible with those of other manufacturers, who, in turn, clone IBM machines.

1981: Xerox Start System introduces the concept of windows, icons, and menus.

1984: Apple Computer, Inc., introduces the Macintosh, an early commercially popular and user friendly microcomputer.

Late 1980s: Chip memory increases to 200-million characters. The optical microchip uses light instead of electricity

to transmit data. Today, optics are setting a 1990s trend, as electronics set in previous decades.

While personal computers were moving into the home, supercomputers entered the laboratory. In the mid-1960s Cray and Intel Corp. developed systems with more memory and speed than mainframes had.

And today we have Deep Blue, an affectionate name for an IBM supercomputer that plays an enviable game of chess. Deep Blue, which mastered 200-million chess moves, belongs to a family called *massively parallel computers*. The term refers to computers linked to cooperatively solve multiple aspects of one complex problem. Working at

one-trillion calculations per second, the most advanced massively parallel computer, the teraflop, is changing how engineers work.

In the past, engineers studied a phenomenon one aspect at a time. They churned out endless quantities of raw information that was converted to insight only with great difficulty. Instead of gaining understanding, too often researchers wrestled with too much of a good thing. Massively parallel computers enable scientists and engineers to render useful what had been an information glut. □

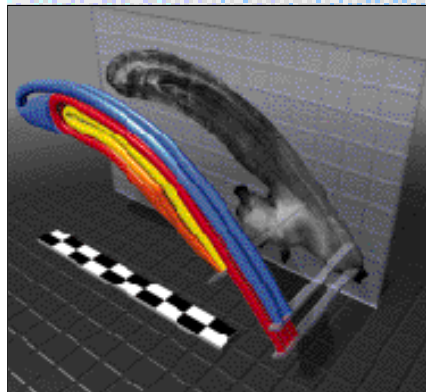
A Walk Through the Simulation Process

Modeling and simulation start with a problem. To solve the problem, which may be very complex, the researcher first measures the object or phenomenon in question.

Measurements — raw data — are then fed into a computer along with instructions that tell the computer what to do with the measurements. An accurate three-dimensional computer image — the model — of the object or phenomenon results. Sometimes the researcher can learn enough by studying the model to gain a new understanding. Other times a simulation must re-enact the problem, during or after which consequences that had been unknown become apparent. Like

eye glasses, the computer is a tool. The brain is still the star.

The following discussion provides a step-by-step walk through two simulations performed on the teraflop computer.



DINOSAUR CREST —
Model showing the interior structures that acted as a resonating chamber.

One simulation solved a 75-million-year-old riddle

How did an extinct dinosaur use its crest? Sandian Carl Diegert worked with paleontology curator Thomas Williamson to solve this problem for the New Mexico Museum of Natural History. Diegert and Williamson

examined a dinosaur fossil to discover the function of a 4-foot-long crest on the animal's head. They used a hospital x-ray machine to scan the fossilized bone and produce measurements fed into the teraflop computer. The resulting computer model revealed that the crest contained air passages. When the scientists studied the crest model for respiratory structures that would prove the dinosaur either warm- or cold-blooded, they found none, but they did find other evidence of warm-bloodedness.

The crest function still in question, the researchers re-enacted on computer what would happen when air passed through tubes and discovered that the crest was a resonating chamber that issued sound.

Digital reconstruction revealed underlying structures that no physical examination ever could. Based on an understanding of certain orchestral wind instruments, Diegert has recreated the call of an animal extinct for 75-million years. □

Another teraflop simulation assessed the damage of a comet colliding with the Earth

How great would the danger be to coastal residents if a comet hit the Atlantic Ocean? Sandian Dave Crawford performed a simulation on the teraflop computer. Crawford used computer codes developed for impact studies of weapons — work

performed to safeguard the nuclear stockpile.

This test represents the first high resolution, three-dimensional simulation of a comet/Earth impact at a 45-degree angle and the first simulation to show the progressive physical changes of air, water, and rock occurring simultaneously and interacting upon one another. Before the teraflop became available, simulations could depict a comet as moving toward the

Earth only at a 90-degree angle.

The test comet is composed of ice and is 0.6 miles in diameter, traveling at 37 miles per second at a 45-degree angle toward the surface of the water. The ocean at the impact site is 3 miles deep. The changing temperature, pressure, and density of air, water, and rock are also fed into the computer. Blue and green represent the different densities of atmosphere. Orange depicts ice (the comet) and water. Red represents the rock seafloor. For size comparison, the scale bar in the lower right shows the New York City skyline in Figure 4. Figures 1, 2, and 3 show slices through a three-dimensional image.

Figure 1: The comet is traveling at 37 miles per second. The changing physics of the air, water, and rock are recreated as they would actually occur.

Figure 2: Just before impact, the comet drills a hole through the atmosphere. The hole (deep blue) fills with low density, high temperature gases as the comet begins to break apart.

Figure 3: One-point-three (1.3) seconds after impact, the hole in the atmosphere becomes a conduit through which impact materials rise into the atmosphere. The black lines show comet material. The yellow color represents vapor exploding upward as a vapor cavity travels down to the ocean floor.

Figure 4: At 8 seconds after impact, a 30,000-foot-high tidal wave forms. It will, however, diminish to 300 feet high when it

reaches the shore. This figure zeroes in on a small section of the impact.

The comet impact and subsequent explosion would compare to a blast 100,000 times greater than that of Mt. St. Helens. The impact would reach the sea floor, but the water would absorb most of the shock, leaving the rock relatively undamaged. Not so, however, for both Atlantic shores, which would be subjected to significant tidal waves.

The simulation used 1,500 processors and took 48 hours. Using the best equipment available in 1994, a comparable simulation would have taken an estimated 20 days. In the early 1990s the best equipment then available would have produced a simulation in about one year. □

THE STACK OF FOUR IMAGES shows stages in a simulation that studied what would happen if a comet hit the Earth. Five hundred comets and 120 asteroids 0.6 miles in diameter or larger intersect the Earth's orbit. A major collision is predicted to occur every 100,000 years.

Fig. 4
Legend shows the New York City skyline, a 3-mile stretch.

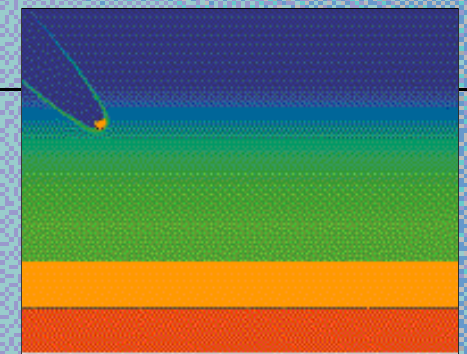


Fig. 1

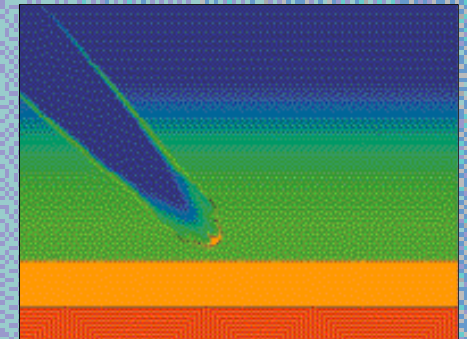


Fig. 2

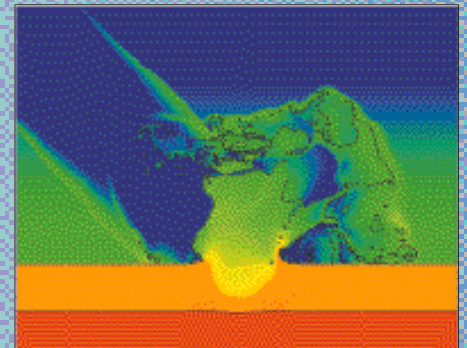
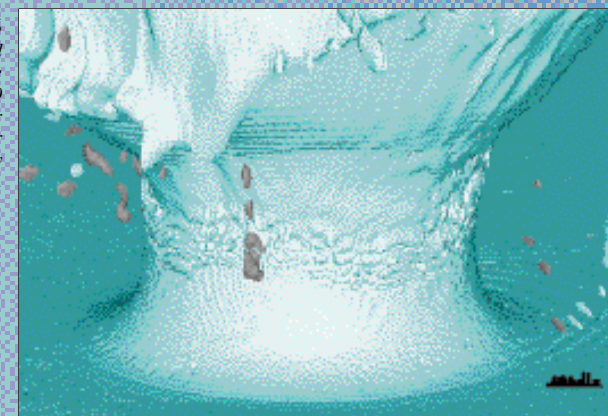
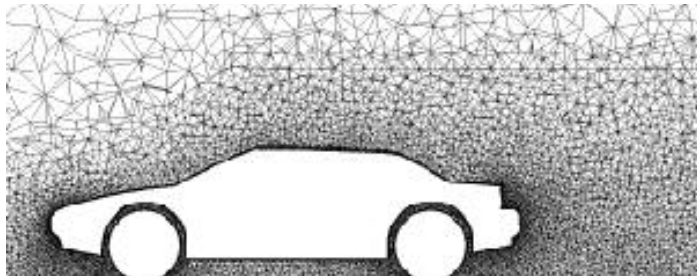


Fig. 3



Suggested Reading: Boslough, Mark B. *Comet crash physics*. Sandia National Laboratories. March 1995. SAND95-0801A.
Williamson, Thomas E., et al. *Inside the complex narial crest of parasaurolaphus (dinosauria, hadrosauridae)*. New Mexico Museum of Natural History and Science, Albuquerque, NM. May 1996.

MARKETS FOR THE NEXT MILLENNIUM



AUTOMATED MESH GENERATION

Automation cuts design time and cost, improves reliability

Modern engineering often relies on simulation of the behavior of parts that the engineer designs. A key step in this process is a technique called meshing. Carried out by computer, meshing breaks an object into small, simple shapes called mesh elements. Together, mesh elements approximate the shape of a part. For flat parts (those stamped from a sheet of metal), the mesh is a collection of lopsided triangles or squares that look like a chicken-wire version of the part. For solid objects, the concept is the same, but the mesh is a collection of irregular tetrahedrons (containing four planes) or bricks.

When the mesh is computed, equations from physics or engineering are applied to each simple mesh element and then solved collectively to determine the behavior of a complicated system. Engineers prefer the square or brick version of a mesh because they lead to more reliable, accurate simulations. But until recently, computing such meshes (for even the simpler case of flat parts) was a difficult job requiring weeks or even months of an engineer's time to guide the computer through the process.

However, Sandia has invented a method that allows the computer to generate flat, quadrilateral meshes without interactive guidance, often in a few minutes. This technology represents an engineering breakthrough and has been honored with several national engineering awards. Also, 10 major U.S. manufacturers — including Ford Motor Co., Chrysler Corp., General Motors Corp., and Goodyear Tire and Rubber Co. — are using this technology routinely.

The benefit to the man on the street, said senior engineer Donald Dewhirst of Ford, is cost savings from solving design problems faster.

Sandia engineers and scientists are working with colleagues in industry to achieve a similar breakthrough for the solid, brick version of the meshing problem. Significant progress is being made. Success here is expected to have a dramatic impact on both Sandia's ability to meet mission goals and the competitiveness of our partners in industry. □

For a fraction of the time real-world tests require, modeling and simulation enable industry to research, design, and test prototypes all on the computer screen

Trial and error has been the engineer's friend — or nemesis — since humans made the first stone tool. Even recently, manufacturers limited product tests to a few affordable and low risk scenarios. Assumptions determined what trials future products would undergo. Trial-and-error product development collected a bounty in time, materials, and sometimes lives.

Those costs and risks are disappearing with modeling and simulation, a technique that uses mathematics to describe phenomena and their behavior under stress — all on the screen of a high performance computer. Modeling and simulation are helping Sandia meet our manufacturing goals: to reduce defects by 90% and to cut manufacturing time and production costs, both by 50%.

The process

A computer model is created by translating features of a car, for example, into equations and data. The computer

then converts these numbers into three-dimensional images — a model — that looks just like the car. The next step is to simulate its behavior under stress.

Historically, the only way to test the effects of stress was to impose stress on the real-world object. The car was crashed, the bomb detonated, the patient operated on. Today, engineers use computers to simulate the crash, detonation, and surgery — a safer, less expensive learning experience.

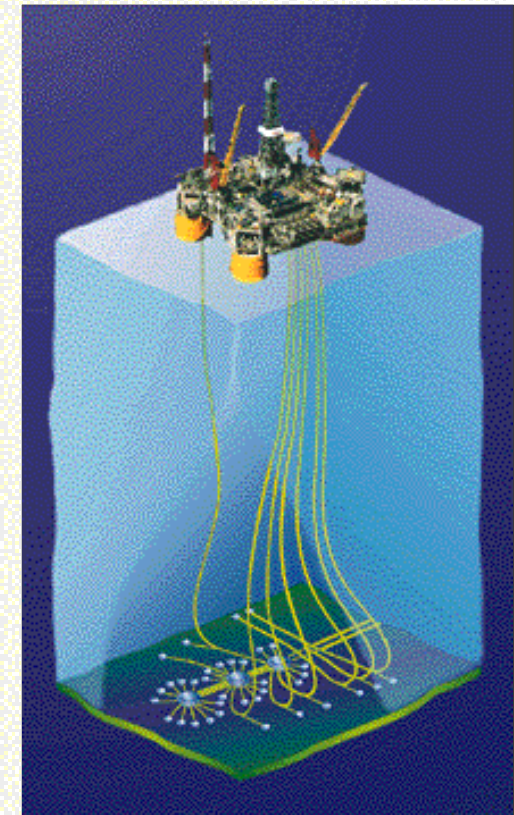
Computer memory and speed are key factors in computer simulation. Working together Sandia and Intel Corp. have set speed and memory milestones. Now manufacturers can duplicate difficult experiments, define complex processes, predict trends, and perform calculations 100 times faster than with previous technologies.

Modeling and simulation enable industry to anticipate dangerous or costly deficiencies and solve problems before developing a product. Pioneered for the space program and applied also to nuclear stockpile stewardship, simulation technology allows fewer or no actual tests that risk lives, cost money, and destroy materials. Simulations can explore nearly all possible scenarios, and resulting products have fewer defects. Industry can modify designs for the most competitive product life cycle, quality, yield, and market price.

The business of engineering

Here are a few examples of how modeling and simulation are affecting industry. (Also see *A Spectrum of Uses*, pages 12 – 16.)

- Rapidly evolving microelectronics technologies require a short design-to-market turnaround time and ways to address the problem of wafer contamination.



Microelectronics manufacturers are applying simulation to meet these challenges.

- Architects and structural engineers can simulate seismic events to predict if structures will withstand stresses.
- In partnership with Sandia, designers for Goodyear Tire and Rubber Co. are simulating how tires work in order to produce affordable tires that behave reliably in all weather conditions.
- The oil and gas industry has become a partner with Sandia to simulate geologic profiles to locate deposits faster and more economically. □

HIGH PERFORMANCE
computing is being used to solve problems such as the effect of ocean currents on offshore drilling and production risers. Modeling is key to preventing serious environmental problems that result if a pipeline breaks.

Suggested reading: Lober, Randy R., Tautges, Timothy J., & Vaughan, Courtenay. *Parallel Paving: an algorithm for generating distributed, adaptive, all-quadrilateral meshes on parallel computers*. Sandia National Laboratories. March 1997. SAND97-0545.

A SPECTRUM OF USES

ECONOMICS: LITTLE PEOPLE, BIG EFFECTS

It's tax time and John Doe, once a corporate manager, is praying for a tax refund. A casualty of foreign competition, John was downsized last fall. Since then, his savings are gone, the house has a realtor's sign out front, and a scratched 1980s minivan is parked in the driveway where a new sport utility vehicle sat before. John's son quit private school, and his daughter is seeking financial aid to finish college.

John *et al* aren't real. Instead they act out their economic dramas in a software program that models

the economy. Sandia physicist Richard Pryor and his team have created Aspen, a software they hope will predict economic trends and do so with unparalleled accuracy. Using one of the world's fastest computers, Aspen forecasts how changes in interest rates, trade policies, legal restrictions, and other worldwide economic events affect individuals and small businesses — and vice versa.

Aspen simulates the goings-on in a city with 1,500 economic entities

(stores, banks, factories, and branches of government) and 10,000 households — all reacting to decisions that range from a renter's choice to buy a home to the Federal Reserve raising the prime interest rate. The bond and real estate markets as well

as trade policies, legal restrictions, and numerous other economic influences are part of the program. The interactive software uses smart agents (such as John Doe above) to respond to situations (such as downsizing), then integrates the

agents' actions with larger economic forces. Aspen reacts to individual situations. Its reactions are not preprogrammed; they evolve. Aspen learns.

Trying to predict the economy is nothing new. Nor is economic modeling by computer. What makes Aspen innovative is that, for the past 40-plus years, models considered only broad economic factors — not the individual household or the mom-and-

(Continued on page 14)

"A systematic sampling scheme (such as Aspen) would have been a good investment to determine how President Clinton's (healthcare) plan would turn out."

Dr. Lawrence Klein
Nobel Laureate in economics

Modeling and simulation were born of national security needs. For space exploration and nuclear stockpile stewardship, risk and expense are extreme, yet safety and reliability are paramount.

In 1963, the United States implemented a treaty to ban all nuclear tests in the air, outer space, and under water. Yet the arsenal remained. Researchers needed an alternative way to discover the effects of spills, leaks, accidents, and the inevitable consequences of time.

Rudimentary modeling began with the nuclear age in the 1940s when equations explained abstract ideas and rehearsed catastrophic scenarios. Some years later, computers began to render two-dimensional pictures of plane crashes, bomb blasts, and structural damage. But the comprehensive test ban treaty, combined with space exploration, ensured that a revolutionary technology would develop to maturity, a technology that could — without consequences — virtually recreate worst-case scenarios.

Today Sandia has developed the most powerful computer in the world — the teraflop — to safely re-enact dangerous events in the virtual world of the computer. The resulting simulations yield knowledge and insight that can help prevent these accidents from ever occurring in the real world. Research initially designed to safeguard the nation and encourage nuclear nonproliferation has expanded our understanding of numerous other fields. As a result, modeling and simulation are finding applications in law enforcement, space



THE ALTUS, an unmanned aerial vehicle, developed to measure the sunlight that clouds absorb, reflect, and transmit.

exploration, weather forecasting, civic projects, transportation safety, medicine, and countless other fields.

Everybody talks about the weather; now somebody's doing something about it

The weather holds us captive. In seconds, a twister levels a town. And a rare freeze in Florida means Christmas oranges double in price. But the greenhouse effect and global warming dwarf local weather concerns.

Allied in a major national effort, NASA, the National Oceanic and Atmospheric Administration, and the Department of Energy (DOE) plus others are studying global change.

DOE, in particular, is examining

how clouds heat and cool the atmosphere. Also, DOE is developing models to improve the tools we have to study climate change. Under DOE's Atmospheric Radiation Measurement - Unmanned Aerospace Vehicle (ARM-UAV) program, Sandia is leading a multilaboratory team using an unmanned aircraft to take atmospheric measurements. The aircraft, called the Altus, measures how much sunlight and thermal energy from the Earth a cloud absorbs, reflects, or transmits. The Altus test flight last fall set a record of 26 hours, 11 minutes for unmanned, long-endurance weather reconnaissance.

Meteorologists hope to use the Altus to observe remote sites for prolonged periods and measure cloud properties to

improve the accuracy of global-warming forecasts. Research findings should help policy makers better understand how to limit the human sources of global weather change.

Sandia's exploratory research fund (LDRD) helped originate and define the basic concepts underlying this project; the Department of Defense Strategic Environmental Research and Development Program funded development of instrumentation, measurement techniques, and taking initial measurements; and DOE is now funding this effort under the ARM-UAV program.

(Please turn to page 14)

(Continued from page 12)

pop corner store. Although the ups and downs of individuals significantly affect the economy, the tools to integrate them into the big picture were lacking.

"They neglected distributive income and purchases among families and (small) businesses," said Lawrence Klein, Nobel Laureate in economics, of past modeling techniques. Klein, who is the Emeritus Benjamin Franklin Professor of Economics at the University of Pennsylvania, does economic forecasting and uses sample surveys of people and businesses.

A nation as big as the United States has so many families and businesses, sophisticated and powerful hardware and software are needed for economic modeling, Klein said.

"Traditionally," said Pryor, "economists tried to solve a whole problem at one time. Aspen looks at each individual (agent) and how he'll react, then integrates what all the agents do. We don't try to control what each one does. We just put them all in a bucket and see what happens." Aspen people get and lose jobs, Aspen banks make loans, corporations merge, and all become wiser for their experiences.

"If a corporation raises the price on goods and the price rise is right, then mathematical instructions in the software reinforce that decision — its correctness allows it to survive, and

other corporations may be deleted," Pryor said. "Things successful breed with things successful and make offspring."

Had Aspen been developed at that time, an ideal problem to test it on would have been President Clinton's proposed healthcare revamp, said Klein, who is a project consultant. "People made quick judgments based on statistics on how doctors, hospitals, patients, and providers would function," he said. "I think they came to inconsistent conclusions. I felt a systematic sampling scheme (such as Aspen) would have been a good investment to determine how President Clinton's plan would turn out."

Other trials might include the flat tax proposed in the last presidential election and the effects of the North American Free Trade Agreement.

Banks, businesses, venture capitalists, financial officers, and anyone with an interest in economic trends should find Aspen useful. Pryor and his team have demonstrated Aspen for the U.S. Federal Reserve. Since *World Business*, *Business Week*, *Aviation Week*, and other magazines have featured Aspen software, Pryor has received worldwide inquiries ranging from researchers at the University of Wisconsin to Caracas, Venezuela; from textile industry to auto manufacturers. A patent is pending. □

Suggested Reading: Basu, N., Quint, T., Pryor, R. J. *Development of Aspen: A microanalytic simulation model of the U.S. economy.* Sandia National Laboratories, Albuquerque, NM. February 1996. SAND96-0434.

Pryor, R. J., Basu, N., Quint, T. *Aspen: A microsimulation model of the economy.* Sandia National Laboratories, Albuquerque, NM. May 1996. SAND96-1225A.

(Continued from page 13)

Crash and burn to save lives

Sandia scientists must determine how weapons will react during accidents and then engineer ways to overcome or reduce ill effects. To do this, we use the teraflop computer to simulate many possible catastrophes.

For example, researchers explore what would happen if a plane crashed. What would happen to structures? How fast would the fire spread? How big would it be? The findings are then applied to designing better planes for the future, modifying existing aircraft, and developing strategies to respond to such accidents.

Fire simulations provide insights on thermal, chemical, and mechanical reactions that could trigger a warhead if a plane carrying a nuclear weapon crashed.

Thwarting crime

Gunshots and adrenaline conspire to foil law enforcement officers trying to free a hostage. If they mistakenly shoot the captive, no harm is done in a virtual VRaptor scenario.

VRaptor software permits such situations to be set up in virtual reality and changed on the spot. A law enforcement trainee wears a helmet that tracks head movements and shows the virtual scene as though the trainee were at an actual crime scene. Amid confusion and rapid changes, trainees can rehearse different scenarios to distinguish between hostage and captor, then disable the captors, and free the hostage.

(Please turn to page 16)



CRASH AND BURN — Responsible for the safety, security, and reliability of the nation's nuclear weapons, Sandia uses simulation to analyze the outcomes of nuclear accidents. The DOE Accelerated Strategic Computing Initiative developed the teraflop to model the aging nuclear stockpile, rather than conduct real-world tests. Fire simulations provide insights on situations that could trigger a nuclear mishap.

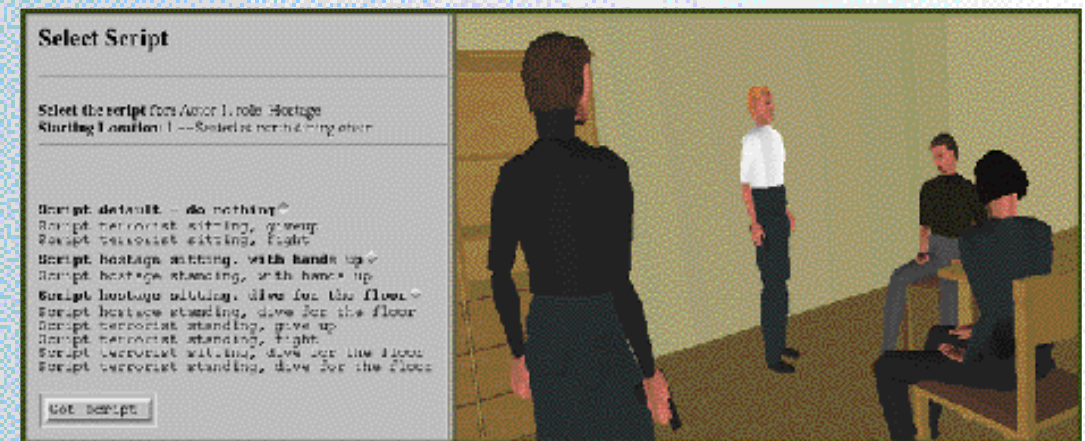
Virtual Reality

Virtual reality is an important tool in simulating and predicting outcomes of otherwise unpredictable situations. But it's not yet the slick scenarios we see on Star Trek where characters physically step into a realm indistinguishable from the real world.

Instead, the term virtual reality refers to an immersive computer environment — such as that created by the VRaptor program — which reacts to the operator's responses. Equipment in a helmet tracks the operator's head movements to determine what the operator sees. The user can participate to a limited extent by moving a wand that tracks hand movements. The operator's actions cause computer reactions, to which the operator reacts again and so on.

For more information: Mora, Carl J. *We crash, burn, and crush: transportation technology programs at Sandia 1978 – 1996.* Sandia National Laboratories, Albuquerque, NM. June 1996. SAND96-1577. (Display at Sandia Credit Union and the National Atomic Museum.)

Suggested reading: Stansfield, Sharon, & Shawver, D. "Using Virtual Reality to Train and Plan Response Actions to Acts of Terrorism." *Proceedings of the SPIE — The International Society for Optical Engineering — Conference on Enabling Technologies for Law Enforcement and Security, November 18 – 22, 1996.* Boston, MA. SPIE. 1996.



VRAPTOR — The menu for the VRaptor program and a virtual image as it appears to the participant in this immersive environment.

Doctoring medicine

Too often medicine becomes a bitter pill. Artificial limbs can make walking again a pain; mammography to detect breast cancer may, through repeated exposure to x-rays, boost a woman's chances of contracting the disease; misreading of x-rays may increase risk as well. And a patient with a brain tumor may venture everything for a tricky surgical cure.

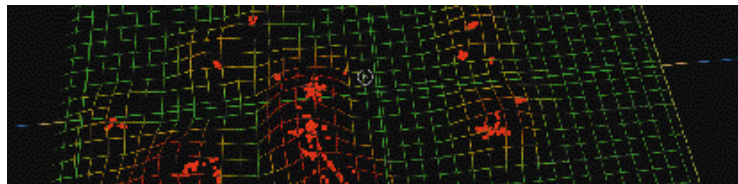
Today powerful computers can reduce the risk and misery involved in some treatments. Working with Johns Hopkins Oncology Center and a major U.S. drug company, Sandia has used supercomputers to make complex calculations that lead to better cancer-fighting drugs. A Sandia – University of Texas collaboration simulated skin and bone surfaces to improve the fit of prosthetics for below-the-knee amputees. Supercomputers are designing better artificial hips, as well. Another project used three-dimensional imaging to detect twice as many breast lesions as mammography does; and these

images better distinguish between tumor, silicone, healthy, and scar tissue than mammograms do. Recent advances in imaging allow brain surgeons to practice on a virtual brain, an exact copy of a real patient's head, thus greatly reducing chances of error. For a closer look at arteries, lesions, and tissue, the surgeon can become a tiny virtual presence, the size of a molecule, and, like Alice *Through the Looking Glass*, enter the brain and travel about.

Experiencing data

Data mapping, a field Sandia is exploring, shapes ideas — literally. Information can be grouped and displayed in a three-dimensional landscape with mountains and valleys (see *Emergent*, vol. 2 no. 1). For example, consider trying to determine how much impact a scientific paper has. An algorithm groups references to the paper. This mathematical representation is translated into an image of a three-dimensional landscape where incidences of heavy citation become mountain peaks — the heavier the citation, the taller the peak. An analyst can then study contours that are invisible as raw data. Data too extensive to understand as numbers shed valuable insight when seen as mountains, ridges, valleys, and islands. □

Suggested Reading: Diegert, Carl, Sanders, J. A., et al. "Practical computer-aided registration of multiple, three dimensional, magnetic resonance observations of the human brain." *Proceedings of the SPIE — The International Society for Optical Engineering*, July 12 – 13, 1995, San Diego, CA. V.2032, SPIE, 1993.



DATA MAPPING displays information (such as the number of documents and their relationship) as a landscape or map. An analyst can then study the map to gain insight not available from raw, unmaped data.



C. E. Meyers, LDRD Manager
Sandia National Laboratories

PERSPECTIVE: But is it alive?

*What is life? It is the flash of a firefly in the night. It is the breath of a buffalo in the winter time. It is the little shadow that runs across the grass and loses itself in the sunset.**

Since a computer won a world-class chess match last year, people have been comparing software to wetware (a.k.a. the brain). But the two don't compare — they complement. Computers help us be better people. Just as the lawn mower makes quick work of the yard so we can spend the afternoon, say, composing music, the computer slogs through calculations, which frees the brain to make discoveries. Conventional wisdom calls the computer a tool.

Yet something human in us wants to build more than a tool. We think we're making strides. Neural networks (numerical models that try to mimic the brain) can be said to learn as the brain learns, by association. Aspen software (discussed on page 12) is an example.

"On a very simple level," said Aspen designer Richard Pryor, "it mimics association. We (humans) have inputs such as sights and sounds. Aspen has much better defined inputs." In other words, Aspen has a cut-and-dried reality. People, however, live in a nebulous, morphing world with no clear boundaries, a world where subtle choices shade outcomes that demand further choices.

Even though the most powerful software — performing a trillion calculations per second — leaves wetware speed in the dust, we know the brain has more "upstairs." It's complex. It's alive.

Typically, software uses computation — a laborious, methodical process — to consider one complicated numerical problem in detail. In comparison, wetware is thought to use association — a chaotic, creative process. The brain also performs the gruntwork to keep the body alive, simultaneously arbitrating the physiological demands of emotions: happiness, greed, curiosity, anxiety, and all the irksome *-isms* that make people quirky. The brain can chew gum and do taxes at the same time.

No computer does that. Yet in true human style, the wetware rallies to keep the dream alive. Every day somewhere on Earth someone advances computer technology. It becomes more like a brain — more like life.

Take Deep Blue, the reigning chess champ, which (or who) recently retired. Here's a machine with a name — as opposed to a make, model, and serial number. Big-name Blue has global celebrity. Blue has an identity — to us. Blue has a purpose — to its designer, IBM. And Blue has distinction — in the eyes of the world — as the first machine to beat a biped at chess. But did Blue get pre-game jitters? Did Blue *hope* to win? Was it *aware* of designers scrutinizing its game?

Will celebrity *spoil* Blue? Does Deep Blue *know* Deep Blue?

Most people agree Blue has yet to get a life. Still, a well understood machine used umpteen thousand processors to compute every move and thus beat the world's most competent human at his own game.

That's not how Blue's opponent played. Former champ Garry Kasparov drew instead from reservoirs of training, strategy, experience, observation, flexibility, and innovation to identify the few best moves and pick one while his brain choreographed how and when to scratch his chin and move chess pieces — and perhaps thwarted urges related to incredulity, confusion, embarrassment, exasperation, and ego. In chess, speed counts, but chess is a pure problem. Unlike life.

What would live machines do?

Being alive — what does it mean? For starters, getting food. To a computer, data and electricity are food, so computers qualify. It means adapting to the environment. Virtual reality programs adapt. Life means replicating. Computer viruses replicate; they grow, spread, contaminate, infect.

So are computers moving toward an animate state or are they just heavy equipment for dirt work? Will machines emerge as individuals? Will they acquire attitude? A sense of who they are? Will they hero-worship newer models, wish to improve their memories? Depending on how you interpret individualism, attitude, self, and intent, some people say they already do. But are they alive? To answer that, we may have to look into ourselves.

Maybe, but will we care?

Life may emerge in silicon as it did in protoplasm — stranger things have occurred — but right now it has a long row to hoe. We understand machines. We can describe them in detail. But life — entangled, messy, morphing life — defies singular description. A biologist calls it one thing. A philosopher another. Engineers and elderly widows each have slants.

But we know it when we see it and when it slips away. As children we felt the loss of blankets and teddy bears. As adults we may feel a twinge when signing cars and houses over to new owners. Inanimate objects; if we care, we do because we associate experiences. But do we feel anything for the brain tool we see, hear, and touch every day? The keys that fit our fingertips? The connections, the chip? If lightning fried our personal computer, would we linger, feeling empty, by its remains and wonder how it could be that the same chunk of plastic was buzzing and warm one second, silent and still the next? When the blue light went out, would we ponder its mortality?

Somehow I doubt it. I'd wager instead we'd mourn — and deeply — the creative thoughts entered since we last hit "save." □

C. E. Meyers, LDRD Manager
Sandia National Laboratories

* *Crowfoot, 19th-century Blackfoot*



SANDIAN PAUL GOURLEY
*examines a laser device that detects
changes in blood cells.*

Technology Update:

Laser device detects, tracks blood disorders

A past issue of *Emergent* (vol. 2 no. 1) covered a revolution in laser technology whereby light performs functions that, in the past, electricity has performed. At the heart of this revolution is a versatile, new kind of laser that allows laser products to be smaller, more durable, and less expensive. We call this laser a VCSEL (pronounced *vix-el*).

In August, a handheld VCSEL device that can detect and track blood disorders was patented. Developed by Sandia and the National Institutes of Health, the biochip detects sickle-cell anemia and cell-structure changes (such as those caused by the AIDS virus) as well as monitors cell growth. The biochip is expected to hasten

analysis and diagnosis of dangerous materials, such as chemicals, in the blood stream.

"It's possible to take a blood sample containing millions of cells and extract information about each cell in a few minutes," said Sandian Paul Gourley, inventor. "If no cell is cancerous, we get a standard light signal. A cancerous cell gives a bright light at different wavelengths."

Gourley's device recently won an R&D 100 Award. Annually *R&D Magazine* recognizes the most promising technologies emerging from industry, universities, and federal laboratories. The *Chicago Tribune* has called the R&D 100 Award the "Oscar of Invention." □